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AQUEOUS SOLUBILITY OF CL-20

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14. ABSTRACT

The Energetics and Warheads Division of the U.S. Army Armament Research, Development and Engineering Center has been involved in the development of CL-20. An aqueous solubility study was performed to better understand the fate and transport of CL-20 through environmental systems.

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INTRODUCTION

CL-20, also known as HNIW (2,3,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane), is a high energy, high density material. Concerns regarding the environmental fate and transport of CL-20 are arising due to its potential introduction into soil and water matrices. Work is currently being conducted to study the fate and transport of CL-20 in soil and water matrices. Determination of solubility characteristics of CL-20 in water is a preliminary task necessary to begin other fate and transport studies. The aqueous solubility of CL-20 was measured over a broad temperature range and the data were fitted to a generalized solubility model.

AQUEOUS SOLUBILITY SETUP

The solubility experiments investigated the effects of temperature on the concentration of CL-20 in the aqueous phase. All tests used un-ground CL-20 manufactured by ATK Thiokol Propulsion, Brigham City, Utah. The aqueous solubility of CL-20 was measured at temperatures ranging from 4 to 69°C. Solutions were prepared by adding excess amounts of the solid compound (0.15 g) in flasks containing deionized water (300 mL). Experiments were conducted in a water bath and the temperature was controlled within ±0.5°C. A three-blade propeller rotated by an overhead lab stirrer (Stirpak model 4554-10, Cole Parmer) was used to stir the mixture at 150 rpm. Once thermodynamic equilibrium was established at a given temperature, three samples (2 mL each) were withdrawn with a syringe, filtered through 0.2 μ polypropylene filters (Whatman Puradisc 25-PP) and immediately diluted with acetonitrile (1:1 by volume) to avoid precipitation. To overcome CL-20 adsorption losses during filtration, it was necessary to discard the first 0.5 mL of the filtered samples. To avoid re-crystallization of CL-20, all the hardware used for sampling and filtration was equilibrated at the test temperature.

RESULTS AND DISCUSSION

Aqueous solubility data for CL-20 at 12 temperatures are presented in table 1 and plotted in figure 1. The solubility equation used to fit the curve is generally used for compounds that do not ionize or dissociate in solution and where the solid phase in pure. The equation is

$$Ln(x) = A + \frac{B}{T} + CLn(T) \tag{1}$$

where

$$A = -Ln(\gamma) + \frac{\Delta H_m}{RT_m} - \frac{\Delta C_p}{R}\{Ln(T_m) - 1\} \tag{2}$$

$$B = \frac{\Delta C_p}{R} T_m - \frac{\Delta H_m}{R} \tag{3}$$

$$C = \frac{\Delta C_p}{R} \tag{4}$$

and where x is the solubility expressed in mole fraction at the prevailing absolute temperature T(°K). The correlation constants A, B, and C obtained by non-linear analysis of the solubility data versus temperature data (R^2=0.9991) are -511.12, 19,063.26, and 75.76, respectively.

The results show that CL-20 solubility increases with temperature. There is about a 17.5-fold increase in solubility as temperature rises from 4 to 69°C. At ambient temperature, the solubility of CL-20 was found to be 4.33 mg/L. The aqueous solubility of CL-20 is significantly lower than that of RDX.

Table 1
Aqueous solubility of CL-20 as a function of temperature

Temperature (°C)	Solubility of CL-20	
	(mg/L)	Mole fraction
4	2.27 (±0.09)	$9.33\ 10^{-8}$
19.5	3.11 (±0.06)	$1.41\ 10^{-7}$
25	4.33 (±0.04)	$178\ 10^{-7}$
30	5.46 (±0.02)	$2.26\ 10^{-7}$
35	6.69 (±0.01)	$2.86\ 10^{-7}$
39	8.10 (±0.06)	$3.33\ 10^{-7}$
45	11.30 (±0.25)	$4.64\ 10^{-7}$
50	14.16 (±0.47)	$5.82\ 10^{-7}$
55	17.37 (±0.17)	$7.14\ 10^{-7}$
60	23.98 (±0.41)	$9.85\ 10^{-7}$
65	32.36 (±1.03)	$1.33\ 10^{-6}$
69	39.68 (±0.25)	$1.63\ 10^{-6}$

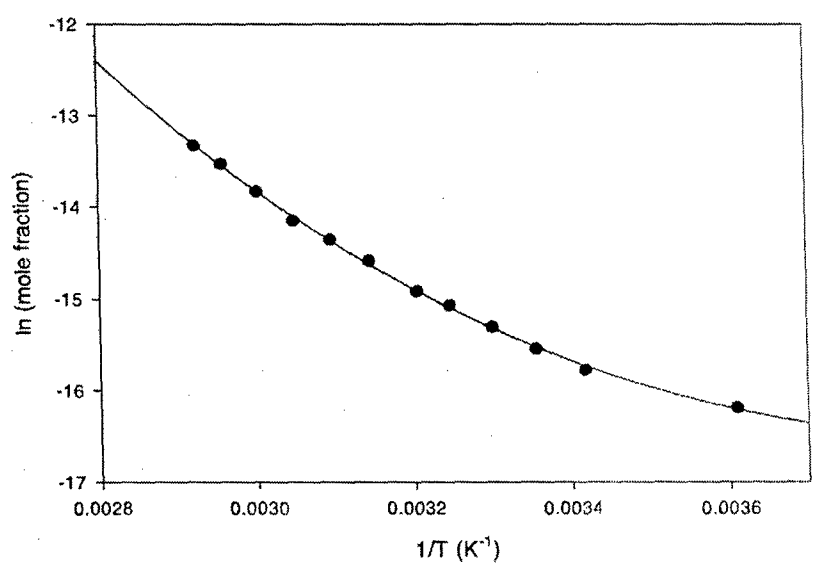

Figure 1
Solubility of CL-20 expressed in mole fraction as a function of temperature
(• experimental data and --- equation 1 fitted to the data)

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